Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36.

TITLE: BIRCH'S LAW AND THE PROPERTIES OF HIGH TEMPERATURE FLUID METALS

LA-UR--87-2921

DE87 014744

AUTHOR(S): J. W. SHANER

SUBMITTED TO: 1987 EHPRG CONFERENCE, AUGUST 25-27, 1987, POTSDAM, DDR

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes.

The Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy





BIRCH'S LAW AND THE PROPERTIES OF HIGH TEMPERATURE FLUID METALS

J. W. Shaner

Los Alamos National Laboratory*
Los Alamos, New Mexico, 87545, USA

Abstract

By comparing acoustic velocities in fluid metals over a very wide range of densities we have established Birch's Law as an approximate representation over the entire liquid range. For a given liquid metal the acoustic velocity is close to linear in density, with a slope determined by the atomic weight. The measurements include isobaric expansion to less than half normal density, ultrasonics on molten metals at 1 atmosphere, and shock-melted metals to greater than twice normal density. We also find unusual behavior of the Gruneisen gamma, which can be explained in terms of simple fluid models.

1. INTRODUCTION

In an attempt to identify what materials lie deep in the earth from seismic velocities, Birch proposed an empirical law that bulk and elastic wave velocities should scale linearly with density and inversely as the square root of the atomic weight. This law was based on elastic constant measurements on rocks to 10 kbar, representing a density change of only 10%, and some early shock wave data from which rarefaction velocities were calculated or measured. Since Birch's original work, several people have tried to explain the linear density dependence as an approximation over a limited density range to more general solid state models. For example, for a normal mode of a simple solid the acoustic wave dispersion relationship is $\omega = ck$, where c is the wave velocity. Since the k vector scales as the reciprocal of the interparticle spacing, $\partial \ln k/\partial \ln \rho = 1/3$. Using the mode gamma definition of Gruneisen's gamma, $\partial \ln \omega/\partial \ln \rho = \gamma$, one has

$$\frac{\partial \ell \, \text{nc}}{\partial \ell \, \text{np}} = \gamma - 1/3 \quad , \tag{1}$$

which integrated becomes

$$c = A\rho^{\lambda}$$
 , (2)

^{*}This work performed under the auspices of the U.S. Department of Energy.

where $\lambda = \gamma - 1/3$. Since γ is generally in the range 1-2 for most simple solids, λ should be around 1.

Over the past few years we have used the optical analyzer technique to measure the pressure at which shocked materials lose their ability to support longitudinal elastic waves. At higher shock pressures, a release wave moves into a fluid-like material at the bulk wave velocity. Above the shock melting pressure we then have measurements of the acoustic velocity of the fluid. New data for liquid lead, obtained by this technique, are presented by Boness, et al.

Another method of measuring thermodynamic properties of fluid metals is the isobaric expansion experiment (IEX). In this experiment, a metal wire is heated in a gas pressure vessel quickly enough so normal hydrodynamic instabilities play no role in the heating dynamics, but slowly enough so that isobaric conditions apply, and the electrodynamic skin effect is insignificant. The function of the gas pressure is to stabilize a homogeneous fluid phase over the widest density range possible. After heating the wire to 5000-10,000 K in several tens of microseconds, we often find a stable liquid column for 10 microseconds, during which time we can perform detailed optical pyrometry or an acoustic velocity measurement.

The acoustic velocity measurement consists of a stress pulse induced by a Q-switched ruby laser pulse of ~0.1 J in 20 nsec, focussed to a spot roughly 0.1 mm on the central portion of the fluid column. This pulse propagates at the bulk sound velocity across the diameter of the wire and initiates a stress wave in the gas at a point diametrically opposite from the laser focal spot. The gas stress wave is detected by Schlieren photography with a streak camera. The velocity is simply the diameter divided by the time interval between the exciting laser pulse and the initiation of the gas stress wave. This technique has allowed us to make measurements of acoustic velocity in lead, for example, expanded to almost one third normal density.

The combination of acoustic velocity and a track on the equation of state (EOS) surface in the form of a (P,V,T) isobar, or a Hugoniot, allow one to determine two orthogonal derivatives of the EOS. Swenson, at al. show how to obtain the Gruneisen gamma,

$$\gamma = V \left(\frac{\partial P}{\partial E} \right)_{V} , \qquad (3)$$

from the Hugoniot and acoustic velocity. This derivative is, up to a simple metric, orthogonal to the isothermal bulk modulus. With isobaric expansion data, one can obtain the Gruneisen gamma from

$$Y = \frac{\partial V}{\partial H} \Big|_{P} c^{2} , \qquad (4)$$

where H is the enthalpy, the electrical energy input at constant pressure, and c

where H is the enthalpy, the electrical energy input at constant pressure, and c is the acoustic velocity. Temperature measurements along the Hugoniot permit an experimental determination of the isothermal bulk modulus by straightforward but tedious arithmetic. Along the isobar, the isothermal bulk modulus, B_T , can be determined from

$$C_p = C_v + \alpha^2 VTB_T$$

and

$$c^2 = VB_T C_p/C_V , \qquad (5)$$

where α is the volume thermal expansion coefficient and $C_{p,V}$ are the heat capacities. Everything is measured experimentally in Eq. (5) except C_V and B_T .

2. EXPERIMENTAL DATA

We present acoustic velocity data for expanded liquid lead and tantalum in Fig. 1.

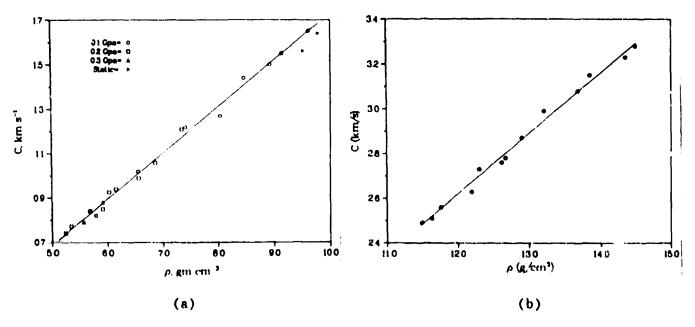


Figure 1. Acoustic velocity in heated, expanded liquid metals: a) lead (Ref. 8); b) tantalum (Ref. 10).

The lead data at high temperatures and expansions show no pressure dependence. Since the P,V isobars separate at high temperatures we can say that the acoustic velocity is only weakly temperature dependent, at least at high expansions. These isobaric expansion data show the normally observed linear dependence of

acoustic velocity on density, but to much higher expansions than are usually obtained for metals.

The combination of data presently available for acoustic velocity in metals in expansion, shock compression, and at the one-atmosphere melting point is shown in Fig. 2, including the recent data of Boness, et al. The N2 data are from Monte Carlo calculations. The change of slope in the Pb data from expansion to compression is well outside experimental error. It is important to realize that in the shock compression regions the density derivative of the temperature is positive, while it is negative in the expansion region, so any temperature dependence might tend to skew the data with respect to a straight line fit. In principle one should plot isotherms of c vs. density, but under the extreme energy density conditions of these experiments, well defined thermodynamic data are limited.

In Fig. 3 we show the other part of Birch's law for fluid metals - that the sound velocity should scale as the reciprocal square root of the atomic mass. This relationship works well for metals in the same column of the periodic table, which therefore have similar core structures. The offset of one metal group from another has no such simple interpretation yet.

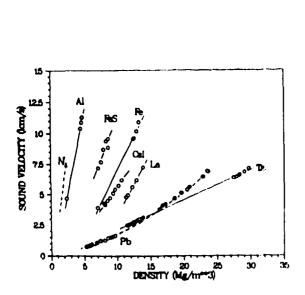


Figure 2. Density dependence of sound velocity for liquid metals.

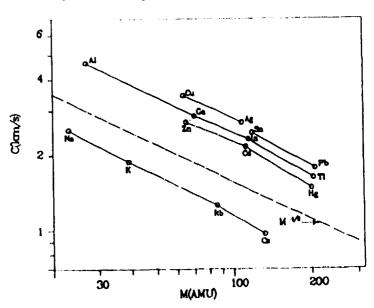


Figure 3. Acoustic velocity of liquid metals as a function of atomic mass. The thermodynamic state is the 1 atmosphere melting point in all cases (Ref. 13).

Gruneisen's gamma shows unexpected behavior for Pb when plotted against density alone, as is shown in Fig. 4. The data of Boness, et al. 0 , show $\rho\gamma$ to be weakly density dependent. On the other hand, the IEX data show γ/ρ to be roughly constant. Therefore, the slope of $\gamma(\rho)$ changes sign around normal density in this representation.

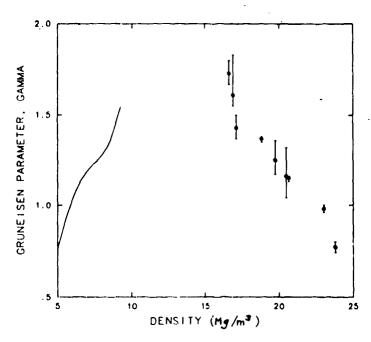


Figure 4. Density dependence of Gruneisen's Gamma for liquid lead.

3. DISCUSSION

The data of Fig. 2 show that the Birch's law suggestion that c is linear in density works reasonably well, even over a density range of three to five, for metals in the liquid range. The average slopes decrease monotonically with atomic mass. At low densities the linearity must break down as one approaches the ideal gas limit, which is independent of density.

We should comment that the display of c and γ vs. density alone is somewhat misleading, since the temperature varies dramatically along these curves. For example, one can prove rigorously that the density derivative of c along the Hugoniot must be greater than or equal to the same derivative along the isobar, which leads to some of the curvature observed when combining isobaric with shock data. If isotherms were plotted, we might expect an even better representation of Birch's law.

For a linear shock velocity vs. particle velocity, $U_S = C + SU_P$, the pressure derivative of the isentropic bulk modulus is given by B' = 4S-1. Thus, for a simple two parameter equation of state, B_S should scale like density to the 4S-1 power, or

$$c = (B_{S/\rho})^{1/2} \sim \rho^{(2S-1)}$$
 (6)

Since most Hugoniots have S between 1 and 1.5, one expects c to scale between linear and quadratic in density, at least in the compression range. Our data show that this scaling extends to significant expansions as well. The curious

density dependence of gamma can be explained simply by a temperature dependent γ in the fluid phase. In fact, using the soft sphere model, which has been applied to the IEX data, ¹⁴ one obtains an explicitly temperature dependent γ , and the observed shape of the $\gamma(\rho)$ curve. ¹⁵ The explicit temperature dependence of γ must be included for any accurate calculation of the adiabatic gradient, in a convecting fluid, for example. Recognition of an explicitly temperature dependent γ in the liquid is also of particular importance in calculating isothermal compression curves from Hugoniot data extending well into the liquid.

REFERENCES

- 1. F. Birch, Phys. Earth and Planet. Interiors 1, 141 (1968).
- 2. F. Birch, J. Geophys. Res. <u>65</u>, 1083 (1960).
- 3. F. Birch, Geophys. J. Royal Astron. Soc. 4, 295 (1961).
- 4. T. J. Shankland, J. Geophys. Res. 77 3750 (1972), D. H. Chong, Science 177, 261 (1972), and O. L. Anderson, J. Geophys. Res. 78, 4901 (1973).
- 5. R. G. McQueen, J. W. Hopson, and J. N. Fritz, Rev. Sci. Inst. <u>53</u>, 245 (1982).
- 6. D. A. Boness, J. M. Brown, and J. W. Shaner, Proceedings of the 1987 APS Topical Conference on Shock Waves in Condensed Matter, Monterey, CA, July 20-23, 1987.
- G. R. Gathers, J. W. Shaner, and R. L. Brier, Rev. Sci. Inst. 47, 471 (1976).
- 8. R. S. Hixson, M. A. Winkler, and J. W. Shaner, Physica 139 & 140B, 893 (1986).
- 9. C. A. Swenson, J. W. Shaner, and J. M. Brown, Phys. Rev. B34, 7924 (1986).
- 10. R. S. Hixson, M. A. Winkler, and J. W. Shaner, High-Temp. High-Press. 18, 635 (1986).
- J. W. Shaner, in Thermal Expansion 6, I. P. Peggs, ed. [Plenum Press (1979) 69].
- 12. R. LeSar, private communication.
- 13. G.M.B. Webber and R.W.B. Stephens in "Physical Acoustics," vol. IV B, W. Mason, ed. Academic Press, NY, 1968.
- 14. G. R. Gathers, J. W. Shaner, and D. A. Young, Phys. Rev. Lett. 33, 70 (1974).
- 15. J. W. Shaner, to be published.